

# Periodic Orbit Theory

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# 1 Introduction

Semiclassical quantization can be understood as an interference phenomenon. Wave fronts propagate along classical trajectories and build up eigenfunctions if they interfere constructively. In integrable systems tori form a backbone for all classically allowed motions and the conditions for constructive interference yield the well known WKB quantization rule[1, 2, 3]. Furthermore, rather detailed information on wave functions, matrix elements and selection rules can be derived[4, 5].

It appears that for chaotic systems periodic orbits play a role similar to that of tori in integrable systems[6]. Gutzwillers famous stationary phase analysis[7] of the trace of Green's function provides a link between the quantum spectrum and classical periodic orbits. This link has been made explicit for hydrogen in a magnetic field[8, 9] and some molecules[10]: a Fourier transform of the spectrum reveals sharp peaks at the periods of classical periodic orbits. However, periodic orbits are much too numerous to provide a one-to-one connection between individual paths and quantum eigenvalues[1]. Mathematically, this is reflected in the inherent divergence of the formal Gutzwiller trace formula[11, 12]. Experiments on microwave resonances[13] show that such relations hold for more general wave phenomena as well.

Methods to overcome such divergences have been developed in the context of general dynamical systems[14, 15, 16], where invariant sets can be characterized by their periodic points. At the heart of these developments has been the observation that classical periodic orbits are strictly organized, both topologically and metrically, and that this organization can be exploited to rewrite ill behaved sums over periodic orbits in a convergent form. The final result is simple and computationally efficient, sometimes showing faster than exponential convergence[17].

At present, for a succesful application of the program, a symbolic organization of the dynamics is necessary. Because of this requirement, it has been carried out for a few systems only, most notably 2-d billiards formed by three disks or four hyperbolas[18, 19, 20], the anisotropic Kepler problem[19, 21] and collinear Helium[22]. These studies (many relevant contributions are collected in a recent conference proceeding[23]) have demonstrated that indeed the trace formula does yield semiclassical approximations to the eigenvalues. They have also shown that the convergence behaviour can be improved dramatically by imposing a functional equation[19, 20]. The existence of this functional equation is suggested by properties of an  $S$ -matrix approach to quantization[24, 25, 26] and by the existence of a similar relation for the Riemann zeta function[27, 28, 29] and for

Selberg zeta functions on surfaces of constant negative curvature[30, 31], but it has not been possible to derive it within the semiclassical approximation (compare the discussion in Ref. [32])

Another point discussed in these notes concerns the extension of Gutzwiller's theory to include matrix elements as well[33, 34]. In principle, this requires the full Green's function, which can be expressed as a sum over recurrent orbits, i.e., orbits returning to their initial positions in projections, not necessarily in full phase space[35]. It turns out[36] that in the case of sufficiently smooth operators, one can again arrive at expressions involving periodic orbits only. This then establishes a complete link between experimentally accessible spectra and classical periodic orbits.

The key technical step will be to express sums over periodic orbits as products over periodic orbits. Such products are termed 'dynamical zeta functions'[37], in analogy to Riemann's zeta function[38, 39], which can be written as an infinite product over prime numbers,

$$\zeta_R^{-1}(s) = \prod_{\text{primes}} (1 - p^{-s}). \quad (1)$$

Dynamical zeta functions look similar, the product extending over contributions from primitive periodic orbits (labelled  $p$ ),

$$\zeta_{Dyn}^{-1}(s) = \prod_p (1 - t_p(s)). \quad (2)$$

The fact is, though, that the objects one is interested in are the products as given above, almost never the inverses thereof. Thus there is an inverse relationship in the behaviour of the two types of functions. For instance, in accord with one approach to the Riemann hypothesis[39], one would like to identify the zeros of  $\zeta_R(s)$  along the critical line  $s = 1/2 + it$  with eigenvalues of a quantum system. However, dynamical zeta functions  $\zeta_D(s)$  have poles rather than zeros at the positions of the eigenvalues.

The theory will be discussed for two degree of freedom systems only, since they are the at present most interesting class. In many cases, extensions to more degrees of freedom are possible.

The organization of the paper is as follows. In the next section, I will summarize Gutzwiller's theory for the spectrum of eigenenergies and extend it to diagonal matrix elements as well. The derivation of the associated zeta function is given (2.2) and the identification of suitable scaling variables discussed (2.3).

In section 3 tools necessary for the organization of chaos will be discussed: symbolic dynamics (3.1), the connectivity matrix (3.3), the topological zeta function (3.4) and

general transfer matrices and zeta functions (3.5). Although illustrated for the case of hard collisions in a billiard, the symbolic dynamics can be extended to ‘smooth collisions’ in smooth potentials (3.2).

In systems with discrete symmetries, zeta functions factorize into zeta functions on invariant subspaces. This symmetry factorization and the associated reduction in symbolics is discussed in section 4.

The ideas developed here are illustrated for the example of a free particle reflected elastically off three disks in section 5. Methods to find periodic orbits (5.1), the convergence of the trace formula (5.2), the semiclassical computation of scattering resonances (5.3), the convergence of the cycle expansion (5.4) and methods to obtain eigenvalues of the bounded billiard (5.5) are discussed.

The relevant parts of a classical periodic orbit theory are developed in section 6.1, including a discussion of escape rates and the Hannay-Ozorio de Almeida sum rule (6.2).

Finally, the issue of semiclassical matrix elements is taken up again and applications to experiments are discussed.

## 2 Semiclassical periodic orbit theory

Following Gutzwiller[6, 7], a connection between periodic orbits and quantum properties can be derived from a stationary phase evaluation of Feynman’s path integral. Usually, only the trace of Green’s function is evaluated, but as will be shown below, a simple extension allows for the computation of matrix elements as well.

### 2.1 Expressions for $\text{tr } GA$

Starting point is the quantum mechanical expression for the trace of Green’s function times some observable,  $g_A(E) = \text{tr } GA$ . Expanded in the (complete) energy eigenbasis (states  $|n\rangle$  of energy  $E_n$ ), this expression takes on the form

$$g_A(E) = \lim_{\epsilon \rightarrow 0} \sum_n \frac{\langle n|A|n\rangle}{E - E_n + i\epsilon}, \quad (3)$$

so that

$$\rho_A(E) = -\frac{1}{\pi} \text{Im } g_A(E) = \sum_n \langle n|A|n\rangle \delta(E - E_n). \quad (4)$$

Thus  $\rho_A$  has poles at the quantum eigenvalues, with residues given by the matrix elements.

The way to obtain the semiclassical expression for (4) is to consider a semiclassical approximation to the propagator, to Fourier transform to find Green's function and then to take the trace. Technically, since the observable can also depend on momenta, one has to use a phase space representation such as Wigner's function[40, 36].

Contributions to the trace come from two sources: from the very short paths, where the propagator turns into a delta function[41], and from the periodic paths. To evaluate the first part, one uses a Taylor series expansion of the trajectory in powers of time  $t$ , and exploits the smallness of  $t$  in evaluating integrals[43, 44]. This then gives a smoothly varying contribution to  $g_A$ ,

$$g_{A,0} = \int \frac{d\mathbf{p}d\mathbf{q}}{h^N} \delta(E - H(\mathbf{p}, \mathbf{q})) A(\mathbf{p}, \mathbf{q}), \quad (5)$$

i.e. the average of the observable over the energy shell.  $N$  is the number of degrees of freedom. Higher order corrections, similar to the boundary and curvature corrections to Weyl's law for billiards, can also be calculated[42, 43, 44].

The second part is obtained by approximating the propagator as a superposition of contributions from all paths. After a stationary phase evaluation of the Fourier transform one obtains the oscillatory part of Green's function[41],

$$G_{osc}(\mathbf{q}', \mathbf{q}; E) = \frac{1}{i\hbar(2\pi i\hbar)^{(N-1)/2}} \sum_{paths} |D_S|^{1/2} e^{iS_p(E)/\hbar - i\pi\nu'_p/2}, \quad (6)$$

where the sum extends over classical paths  $p$  connecting  $\mathbf{q}_1$  and  $\mathbf{q}_2$  at a fixed energy  $E$ , irrespective of the time it takes;  $S_p$  is the classical action  $\int \mathbf{p} d\mathbf{q}$ ,

$$D_S = \det \begin{pmatrix} \frac{\partial^2 S_p}{\partial \mathbf{q}' \partial \mathbf{q}} & \frac{\partial^2 S_p}{\partial E \partial \mathbf{q}} \\ \frac{\partial^2 S_p}{\partial \mathbf{q}' \partial E} & \frac{\partial^2 S_p}{\partial E^2} \end{pmatrix} \quad (7)$$

is the determinant of second derivatives and the index  $\nu'_p$  counts the number of caustics on the energy shell.

The next step is to take the trace of  $GA$ ,

$$g_A = \int d^N \mathbf{q} G(\mathbf{q}, \mathbf{q}; E) A(\mathbf{q}), \quad (8)$$

where for simplicity an observable depending on positions only has been substituted. In spirit with the semiclassical nature of the entire calculation one would also like to evaluate this integral in stationary phase. This is possible, if  $A$  varies slowly on the scale of a wavenumber. The calculation then continues very much as in Gutzwiller's case[7, 36].

The phase is stationary if the final and initial momenta coincide, which is the condition that the trajectory be periodic. In the neighbourhood of every closed path a coordinate

system with  $q_1$  along the path and  $q_2, \dots, q_N$  perpendicular to it may be introduced. Using the factorization of the determinant  $D_S$  and the fact that up to second order in the deviations from the trajectory the action only depends on the stability matrix of the classical path, one finds

$$\frac{1}{(2\pi i\hbar)^{(N-1)/2}} \int dq_2 \cdots dq_N |D_{S_p}|^{1/2} e^{iS_p(\mathbf{q})/\hbar - i\nu'_p\pi/2} = \frac{1}{|\dot{q}_1| |\det(M_p - 1)|^{1/2}} e^{iS_p/\hbar - i\mu_p\pi/2}. \quad (9)$$

where  $S_p$  is the action along the periodic orbit,  $M_p$  is the stability matrix around the orbit and the phase shift  $\mu_p$  is the Maslov index of the periodic orbit[45].

Since the stability matrix is independent of the position along the path, there remains the integral  $\int dq_1 A(\mathbf{q})/\dot{q}_1$ , which by  $dq/\dot{q} = dt$  may be written as a time integral over one period. Allowing for multiple traversals of a periodic orbit, we finally find for the contribution of one periodic orbit to  $g_{A,osc}$ ,

$$g_{A,p} = \frac{-i}{\hbar} A_p \sum_{r=1}^{\infty} \frac{e^{(iS_p/\hbar - i\mu_p\pi/2)r}}{|\det(M_p^r - 1)|^{1/2}}, \quad (10)$$

with  $A_p$  the integral of  $A$  along the orbit.

Combining the smooth part (5) with the contributions from all periodic paths, one finds

$$\begin{aligned} \rho_A(E) &= -\frac{1}{\pi} \text{Im tr } g_A(E) = \rho_{A,0}(E) + \sum_p \rho_{A,p}(E) \\ &= \int \frac{d\mathbf{q}d\mathbf{p}}{h^N} A(\mathbf{q}, \mathbf{p}) \delta(E - H(\mathbf{q}, \mathbf{p})) \\ &\quad + \text{Im} \frac{i}{\pi\hbar} \sum_p \sum_{r=1}^{\infty} \frac{A_p}{|\det(M_p^r - 1)|^{1/2}} e^{(iS_p(E)/\hbar - i\pi\mu/2)r} \end{aligned} \quad (11)$$

where

$$A_p = \int_0^{T_p} dt A(\mathbf{q}_p(t), \mathbf{p}_p(t)). \quad (12)$$

In the final formula general observables  $A(\mathbf{p}, \mathbf{q})$  have been admitted. The momentum  $\mathbf{p}(t)$  is then fixed to be the momentum along the path at  $\mathbf{q}(t)$ . The average of the observable over one period of the classical trajectory  $(\mathbf{p}(t), \mathbf{q}(t))$  is  $A_p/T_p$ . The key requirement, beyond the applicability of a semiclassical approximation, is that the observable be sufficiently smooth. Otherwise a steepest descent approximation to all integrals has to be used. From the above discussion (eq (4)) one expects this expression to show poles at the (semiclassical) eigenvalues, the residues being the matrix elements.

## 2.2 Selberg's and other zeta functions

For the density of states the operator  $A = 1$  and thus  $A_p = T_p$ . Then the contributions from periodic orbits to (11) may be rewritten as the logarithmic derivative of an infinite product over periodic orbits[46], similar to the Selberg zeta function[47] in the theory of geodesic motion on surfaces of constant negative curvature[30].

With  $A = 1$  and  $A_p = T_p$  the period, the contribution from periodic orbits to (11) can be written

$$R_{A,osc} = \frac{i}{\pi\hbar} \sum_p \sum_{r=1}^{\infty} \frac{T_p}{|\det(M_p^r - 1)|^{1/2}} e^{(iS_p/\hbar - i\mu_p\pi/2)r}. \quad (13)$$

The degrees of freedom enter in the size of the linearization perpendicular to the orbit. For a two degree of freedom system,  $M_p$  is a  $2 \times 2$  matrix of determinant one. If the orbit is unstable, the eigenvalues are  $\Lambda_p$  and  $1/\Lambda_p$ . The denominator can then be expanded in a geometric series[48],

$$|\det(M_p^r - 1)|^{-1/2} = |\Lambda_p|^{-r/2} (1 - 1/\Lambda_p)^{-1} = \sum_{j=0}^{\infty} |\Lambda_p|^{-r/2} \Lambda_p^{-jr}, \quad (14)$$

so that

$$R_{A,osc} = \frac{1}{\pi\hbar} \sum_p \sum_{j=0}^{\infty} \sum_{r=1}^{\infty} T_p \left[ e^{iS_p/\hbar - i\mu_p\pi/2} |\Lambda_p|^{-1/2} \Lambda_p^{-j} \right]^r. \quad (15)$$

Upon summing on  $r$  one finds

$$R_{A,osc} = \frac{1}{\pi\hbar} \sum_p \sum_{j=0}^{\infty} \frac{T_p t_p^{(j)}}{1 - t_p^{(j)}}, \quad (16)$$

where  $t_p^{(j)} = e^{iS_p/\hbar - i\mu_p\pi/2} |\Lambda_p|^{-1/2} \Lambda_p^{-j}$ . Using the relation  $T_p = \partial S_p / \partial E$ , one can write the quotient in (16) as a logarithmic derivative,

$$R_{A,osc} = -\frac{1}{\pi} \sum_p \sum_{j=0}^{\infty} \frac{\partial}{\partial E} \log(1 - t_p^{(j)}), \quad (17)$$

so that finally

$$R_{A,osc} = -\frac{1}{\pi} \frac{\partial}{\partial E} \log Z(E) \quad (18)$$

with the Selberg zeta function[47, 46]

$$Z(E) = \prod_{j=0}^{\infty} \prod_p (1 - e^{iS_p/\hbar - i\mu_p\pi/2} |\Lambda_p|^{-1/2} \Lambda_p^{-j}). \quad (19)$$

Deriving zeta functions for the other traces involving matrix elements requires a little trick and will be postponed until later (section 7.1).

Depending on ones application, it sometimes is convenient to think of (19) as an infinite product of dynamical zeta functions,  $Z = \prod_j 1/\zeta_j$  with

$$1/\zeta_j = \prod_p (1 - e^{iS_p/\hbar - i\mu_p\pi/2} |\Lambda_p|^{-1/2} \Lambda_p^{-j}). \quad (20)$$

The leading order term  $1/\zeta_0$  is Gutzwillers original approximation[7, 48], obtained by replacing the determinant in the denominator by the dominant eigenvalue. The discussion of convergence (section 5.2) will reveal that indeed this first term is the dominant one. All other zeta functions converge absolutely and therefore cannot give eigenvalues or resonances near the real energy axis[49].

## 2.3 Scaling variables

In general, the actions of periodic orbits are complicated functions of energy[50]. If the Hamiltonian describing the system has scaling properties, e.g. if it is a sum of squares of the momenta plus a homogeneous potential,  $V(\lambda\mathbf{x}) = \lambda^\kappa V(\mathbf{x})$ , then by a virial theorem, the action scales with energy like

$$S(E) = \frac{2\kappa E_0}{(2+\kappa)} T(E_0) \left( \frac{E}{E_0} \right)^{(2+\kappa)/2\kappa}, \quad (21)$$

where  $E_0$  is some reference energy and  $T$  the period. It thus becomes linear in the variable

$$k = \left( \frac{E}{E_0} \right)^{(2+\kappa)/2\kappa}. \quad (22)$$

In the limit of a billard,  $\kappa \rightarrow \infty$ ,  $k$  is essentially the usual wavenumber. Because of the simple linear scaling of actions with  $k$ , one can use a Fourier transform in this variable to uncover the periodic orbit structures[51, 9].

Such scaling Hamiltonians are exceptional. However, in the limit of small  $\hbar$  one can expand the action to first order in energy around a reference energy  $E_0$ , viz.  $S(E) = S(E_0) + T(E_0)(E - E_0)$ . In this limit it is possible to identify an energy interval which is classically small (the properties of periodic orbits change little) but semiclassically large (the interval contains many quantum eigenvalues). Then approximately  $E$  itself is a good scaling variable. Formally, this is equivalent to consider the eigenvalues as a function of  $\hbar$  for fixed classical energy, as used e.g. in the derivation of the spectral statistics of integrable systems[52].

### 3 Organizing chaos

In this section I provide the necessary formal background on symbolic dynamics, transfer matrices and cycle expansions. These tools are important in developing the theory of zeta functions and their cycle expansions. Eventually, one might hope to overcome these limitations.

#### 3.1 Symbolic dynamics

The paradigmatic example of randomness is a coin toss[53], which, at least in principle, yields as its outcome a string of heads and tails, with no correlations between consecutive events. Thus all strings are possible and equally likely. In a chaotic dynamical system, one can find similar behaviour[54, 55, 37, 56]: first dynamics is reduced to a discrete map using a Poincaré surface of section. Then certain regions in this section are assigned ‘heads’ and ‘tails’. Depending on where a trajectory crosses the surface of section, it will map out a string of heads and tails, and different trajectories will map out different strings. As discussed in MacKay’s lecture, such a construction is generically possible in the vicinity of a homoclinic crossing[57, 58]. Different from the ideal coin tossing experiment, the dynamical coin is loaded: the probability of occurrence of a given symbol is determined by the dynamics and need not be the same for all symbols.

For a certain class of systems it seems possible to extend this symbolic dynamics to all relevant regions of phase space. Specifically, for three or four disks arranged in a plane so that all lines connecting any two disks are possible (and not shaded by a third disk), one has a unique labelling of *periodic* orbits by disk visitation sequences[59, 60] (see Fig. 1). As the disks are moved closer together to form a bounded system, orbits disappear because of shading by one of the disks[61]. Nevertheless, one still seems to be able to label all trapped periodic orbits uniquely by a string of symbols.

Here we focus on the three disk system, which is somewhat simpler than the four disk billiard relevant for hydrogen in a magnetic field[45]. In both systems, every trajectory can be labelled by the disk visitation sequence. The set of labels assigned to the disks is called the *alphabet* (here:  $\{1, 2, 3\}$ ), any string formed from them a *word* (the trajectory shown in Fig. 1 could be labelled by the word 1231312). Evidently, a particle cannot bounce off the same disk twice, so that repetitions of the same symbol are prohibited. This exclusion of  $\dots 11 \dots$ ,  $\dots 22 \dots$  and  $\dots 33 \dots$  is a typical example of a *grammar rule*.

The way in which infinite sequences specify periodic orbits is reminiscent of the same

construction in the horseshoe map[57, 58]. In a typical scattering experiment, the ingoing direction is fixed and the impact parameter varied. Then there will be an entire interval of impact parameters containing trajectories with the same collision future for the next  $n$  collisions. In Fig. 2 the interval in impact parameter leading to collisions with disk 1 is indicated. If the next collision is specified as well, a subinterval is selected. With increasing number of collisions, these intervals shrink to a point: thus, there will be exactly one impact parameter with the prescribed collision sequence. The past of the trajectory depends on the ingoing direction. Repeating then the same procedure for the angle rather than the impact parameter a unique value of both impact parameter and angle will be identified. This construction is very similar to the way in which strings and orbits are associated in the Baker's map[62].

### 3.2 Smooth collisions

The previous discussion might seem confined to billiard models. However, it should be clear that smoothing the discontinuity at the boundaries of the disks a little bit will not change the topology of short orbits. For instance, the potential  $V(x, y) = (xy)^{2/d}$  is equivalent to a billiard bounded by the hyperbola  $xy = 1$  for  $d = 0$  and changes to the quartic oscillator  $x^2y^2$  for  $d = 1$ . Dahlqvist and Russberg[63, 64] have followed periodic orbits from  $d = 0$  (where a code is known) to  $d = 1$  to establish a symbolic coding for the above quartic oscillator. Since the potential becomes more repulsive as  $d$  approaches one, it is difficult to imagine that new orbits are born rather than existing ones destroyed. However, this has to be checked case by case and is not always obvious.

An alternative way has been proposed in Ref. [45, 65]. A characteristic feature of collisions is that a change in orientation in a local coordinate system takes place. One can think of defining the coordinate system using two neighbouring trajectories with parallel velocities. During the collision, they will cross in position space, causing a change in orientation of the local coordinate system.

Related to this change in orientation are self conjugate points, where neighbouring trajectories started with momentum slightly different from the reference trajectory return to it. Then an off diagonal matrix element of the monodromy matrix after a full period  $T$  vanishes,

$$\begin{pmatrix} \delta x_{\perp} \\ \delta p_{\perp} \end{pmatrix} (T) = \begin{pmatrix} m_{xx} & 0 \\ m_{xp} & m_{pp} \end{pmatrix} \begin{pmatrix} \delta x_{\perp} \\ \delta p_{\perp} \end{pmatrix} (0). \quad (23)$$

Regions where one would identify a bounce are bounded by two such conjugate points. As

demonstrated in Fig. 3 this method also works for orbits which are very close in position space and where it is not immediately obvious whether they undergo a collision when approaching the equienergy contour or not.

For the computation of self conjugate points, one can use the linearized equations of motion and the monodromy matrix  $\mathbf{M}$ . For a two degree of freedom system, this is a  $4 \times 4$  matrix, which can be obtained by integrating 16 first order differential equations. Two eigenvalues of  $\mathbf{M}$  after a full period are equal to one, due to the fact that both a shift along the orbit and a shift out of the energy shell will be preserved. The interesting part of  $\mathbf{M}$  is the  $2 \times 2$  matrix  $\mathbf{m}$  describing neighbouring trajectories in a plane perpendicular to the orbit but on the energy shell. As worked out in Ref. [65], it is possible to introduce a coordinate system in which the trivial directions are eliminated and in which closed equations for the  $2 \times 2$  submatrix  $\mathbf{m}$  can be found.

An additional advantage of a definition of a symbolic code in terms of self conjugate points is the close connection to semiclassics. Since the propagator has an amplitude proportional to  $\sqrt{dq_{\perp}(T)/dp_{\perp}(0)}$ , vanishing of the off diagonal element also signals a break down of the semiclassical approximation, the presence of a caustic and a change of the Maslov phase. This close connection between Maslov indices and the symbolic code is important for the cancellation of terms in the cycle expansion (section 5.4).

### 3.3 Connectivity matrix

Given the division of phase space into cells labelled by some alphabet the dynamics enters in form of transitions between different cells. The *connectivity* matrix encodes the information whether it is possible to go from one cell to another or not. In its simplest form, it is defined by

$$T_{i,j} = \begin{cases} 1 & \text{if transition from } j \text{ to } i \text{ is possible} \\ 0 & \text{if it is not possible} \end{cases}, \quad (24)$$

where the indices are letters from the alphabet.

For many applications, especially transfer matrices, a generalization based on refinements of the cells is required. Cells are subdivided and labelled according to the past of trajectories in the subcells. All trajectories which cross the surface of section in a region inside cell  $i_1$ , sharing a common past of crossings at  $i_2, i_3, \dots, i_N$ , define a unique smaller cell which will be labelled  $i_1 i_2 \dots i_N$ . When iterated once, they will cross the surface in any one of the regions with the label  $i_0 i_1 i_2, \dots, i_{N-1}$ , where  $i_0$  can (in principle) be any symbol from the alphabet: the very last symbol is dropped and a new one

added. The connectivity matrix generalizes to one indexed by words  $I = i_1 i_2 \cdots i_N$  and  $J = j_1 j_2 \cdots j_N$ . Since in one iteration only one symbol is dropped and replaced by a new one, the connectivity matrix can have entries at positions with coinciding intermediates only, i.e.  $T_{I,J} \neq 0$  for  $I = a i_1 \cdots i_{N-1}$  and  $J = i_1 \cdots i_{N-1} b$  only.

The number  $N_n$  of allowed strings of length  $n$  is given by the trace of the  $n$ -th power of the connectivity matrix,

$$N_n = \text{tr } T^n. \quad (25)$$

For example, for the case of a complete binary code (symbols 0 and 1, no grammar rule), the transfer matrix is

$$T_{bin} = \begin{array}{cc} & \begin{matrix} 0 & 1 \end{matrix} \\ \begin{matrix} 0 \\ 1 \end{matrix} & \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \end{array}, \quad (26)$$

where the numbers outside the matrix indicate the symbols. One can also define the larger connectivity matrix, acting on pairs of symbols,

$$T_{bin} = \begin{array}{ccccc} & & \begin{matrix} 00 & 01 & 10 & 11 \end{matrix} \\ \begin{matrix} 00 \\ 01 \\ 10 \\ 11 \end{matrix} & \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{pmatrix} \end{array}, \quad (27)$$

It is easily checked that both matrices yield the same strings. The number of strings of length  $n$  that can be formed is  $N_n = 2^n$ . For example, at length 2, the four strings 00, 01, 10 and 11 are possible. Evidently, when periodically continued, 00 and 11 correspond to the fixed points 0 and 1 of length 1 and 01 and 10 describe the same periodic string. The *primitive period*  $n_p$  of a periodic string is the length of the shortest block from which it can be obtained. By cyclic permutation, there are  $n_p$  such blocks.

Thus the total number of strings of length  $n$  can be decomposed into the number  $M_d$  of primitive strings of length  $d$  dividing  $n$ ,

$$N_n = \sum_{d|n} M_d. \quad (28)$$

By Möbius inversion[66], one finds

$$M_d = \frac{1}{n} \sum_{d|n} \mu\left(\frac{n}{d}\right) N_d, \quad (29)$$

where the Möbius function is defined by  $\mu(1) = 1$ ,  $\mu(n) = 0$  if  $n$  contains the square of a prime and  $\mu(n) = (-1)^k$  if  $n$  contains  $k$  prime factors. Some examples are given in table 1.

In case of the three disks with their exclusion rule, the associated connectivity matrix reads

$$T_{3-d} = \begin{array}{c} \begin{array}{ccc} & 1 & 2 & 3 \\ 1 & \begin{pmatrix} 0 & 1 & 1 \end{pmatrix} \\ 2 & \begin{pmatrix} 1 & 0 & 1 \end{pmatrix} \\ 3 & \begin{pmatrix} 1 & 1 & 0 \end{pmatrix} \end{array} \end{array}, \quad (30)$$

the number of strings is  $N_n = 2^n + (-1)^n 2$  and the number of primitive cycles agrees with the one for the binary code, except for  $n = 1$  and  $n = 2$  (see table 1).

### 3.4 Topological zeta function

The number of strings of length  $n$  is given by  $\text{tr} T^n$  and thus dominated by the largest eigenvalue of  $T$ . The inverse of the largest eigenvalue is a zero of  $\det(1 - zT)$ . Using the identity  $\det A = \exp \text{tr} \ln A$  and expanding the logarithm, one finds

$$\det(1 - zT) = \exp \left( - \sum_{n=1}^{\infty} \frac{z^n}{n} \text{tr} T^n \right). \quad (31)$$

If  $T$  is the connectivity matrix, then  $\text{tr} T^n = N_n$ . Using the decomposition (28) one can then replace the sum on  $n$  by one on all primitive periodic orbits  $p$  of symbol length  $n_p$  and their repetitions  $r$ ,

$$\begin{aligned} - \sum_{n=1}^{\infty} \frac{z^n}{n} \text{tr} T^n &= - \sum_p \sum_{r=1}^{\infty} \frac{z^{n_p r}}{n_p r} n_p \\ &= + \sum_p \ln(1 - z^{n_p}), \end{aligned} \quad (32)$$

so that

$$\det(1 - zT) = \prod_p (1 - z^{n_p}). \quad (33)$$

Such products over periodic orbits, formed in analogy to the Riemann zeta function, are called dynamical zeta function[37], or, if they are derived from the connectivity matrix, topological zeta functions. As explained in the introduction they are denoted by  $1/\zeta$ , although it is exactly the product(33) and not its inverse which is studied.

For a complete code on  $m$  symbols, the left hand side is easily evaluated to be  $1 - mz$ . Note the tremendous cancellations this must imply for the infinite product on the right hand side when expanded as a power series in  $z$ ! For example, for a binary code, one has

$$1/\zeta_{bin} = 1 - 2z = (1 - z)^2(1 - z^2)(1 - z^3)^2(1 - z^4)^3 \dots \quad (34)$$

This calculation can be used for the three disks as well. The number of periodic orbits agrees with that for a complete binary coding except for  $n = 1$ , where there is no periodic orbit and  $n = 2$  where there are three rather than just one. Therefore, the topological zeta function for three disks can be obtained from that for the binary case,

$$\begin{aligned} 1/\zeta_{3-d} &= 1/\zeta_{bin} \frac{(1 - z^2)^2}{(1 - z)^2} \\ &= (1 - 2z)(1 + z)^2 = 1 - 3z^2 - 2z^3 \end{aligned} \quad (35)$$

which is still a finite polynomial. If however just one orbit is missing, say one of the fixed points, then the topological zeta function is no longer polynomial,

$$1/\zeta_{pr} = 1/\zeta_{bin} \frac{1}{1 - z} = 1 - z - z^2 - z^3 - \dots \quad (36)$$

Obviously, the leading zero and thus the topological entropy is still two.

### 3.5 Transfer matrices and cycle expansion

Transfer matrices have the same structure as connectivity matrices and the same vanishing elements, but the 1's are replaced by quantities multiplicative along trajectories. They provide the connection to classical statistical mechanics[54, 55, 37, 56] and have been used in semiclassical mechanics first by Gutzwiller[6, 67, 68] in his analysis of the anisotropic Kepler problem. They also figure prominently in Bogomolny's[24, 25] theory of semiclassical quantization. Here, the precise form of *off*-diagonal matrix elements is not so important, since all relevant quantities will be expressed in terms of traces of powers of  $T$ , which involve periodic orbits only. It should be noted that while there is some ambiguity in assigning matrix elements of  $T$ , there is none for periodic orbits and thus traces of  $T^n$ : actions, periods and stability exponents are representation independent.

Entries of the transfer matrix or powers thereof are labelled by the code of the initial and final cells. Diagonal elements are thus associated with contributions from trajectories that start in one cell and return. An increased resolution with its longer code for the cells means that initial conditions for trajectories returning to that cell have to be specified

more precisely, collapsing to a point in the limit of infinite resolution. A primitive cycle of length  $n$  will contribute  $n$  times. If  $p \in (d)$  denotes the different primitive cycles of length  $d$  and  $t_p$  the contribution from cycle  $p$ , then

$$\text{tr } T^n = \sum_{d|n} \sum_{p \in (d)} d t_p. \quad (37)$$

Upon substitution into (31) and manipulations similar to the ones that lead to (33) one finds

$$\det(1 - zT) = \prod_p (1 - z^{n_p} t_p). \quad (38)$$

In general, the transfer matrix will depend on variables (such as the wavenumber in case of the Gutzwiller trace formula) and one is interested in the zeros of (38) as a function of this variable. Therefore,  $z = 1$ . However,  $z$  is extremely valuable as an auxiliary variable when organizing the product. It is only for the final calculation that one puts  $z = 1$ .

The periodic orbits may conveniently be labelled by their symbolic codes. For the case of a complete binary code one thus finds

$$\begin{aligned} \det(1 - zT) = & (1 - zt_0)(1 - zt_1)(1 - z^2 t_{01})(1 - z^3 t_{001})(1 - z^3 t_{011}) \\ & (1 - z^4 t_{0001})(1 - z^4 t_{0011})(1 - z^4 t_{0111})(1 - z^5 t_{00001})(1 - z^5 t_{00011}) \\ & (1 - z^5 t_{00101})(1 - z^5 t_{00111})(1 - z^5 t_{01011})(1 - z^5 t_{01111}) \dots \end{aligned} \quad (39)$$

The cycle expansion is now obtained by factoring out the products and arranging terms in a power series in  $z$ , just as in case of the topological zeta function,

$$\begin{aligned} 1/\zeta = & 1 - zt_0 - zt_1 - z^2[(t_{01} - t_1 t_0)] \\ & - z^3[(t_{001} - t_{01} t_0) - (t_{011} - t_{01} t_1)] \\ & - z^4[(t_{0001} - t_0 t_{001}) + (t_{0111} - t_{011} t_1) \\ & + (t_{0011} - t_{001} t_1 - t_0 t_{011} + t_0 t_{01} t_1)] - \dots \end{aligned} \quad (40)$$

$$= \sum_n c_n z^n \quad (41)$$

The important feature to note is that the contributions  $t_0$  and  $t_1$  from the two fixed points stand isolated but that all others come in groups. In the limit of  $t_p \rightarrow 1$  the connectivity matrix is recovered and as eq (39) shows, the cancellations among all higher order terms are complete. This is the main use of the topological zeta function in this context: it provides a back bone of possible contributions to periodic orbit expressions and shows how they are organized. What remains to be checked is that the coefficients  $c_n$

containing long periodic orbits can be grouped so that cancellations similar to the ones for the topological polynomial actually take place.

Alternatively, one can start from (31) and expand directly in a power series in  $z$ , obtaining expressions reminiscent of a cumulant expansion,

$$\det(1 - zT) = 1 - z \operatorname{tr} T - \frac{z^2}{2}(\operatorname{tr} T^2 - (\operatorname{tr} T)^2) - \frac{z^3}{3}(\operatorname{tr} T^3 - \dots) \dots \quad (42)$$

For instance, the contributions to  $\operatorname{tr} T^2$  are  $(T^2)_{00,00} = t_0^2$ ,  $(T^2)_{11,11} = t_1^2$ ,  $(T^2)_{10,10} = t_{10}$  and  $(T^2)_{01,01} = t_{10}$ . Thus, the second term reduces to

$$\frac{1}{2}(\operatorname{tr} T^2 - (\operatorname{tr} T)^2) = \frac{1}{2}(t_0^2 + t_1^2 + 2t_{01}^2 - (t_0 + t_1)^2) = t_{01} - t_0 t_1 \quad (43)$$

in agreement with the cycle expansion (41).

For the case of three disks with the ternary alphabet with exclusion rules, the zeta function is given by

$$\begin{aligned} 1/\zeta &= (1 - z^2 t_{12})(1 - z^2 t_{13})(1 - z^2 t_{23})(1 - z^3 t_{123})(1 - z^3 t_{132}) \\ &\quad (1 - z^4 t_{1213})(1 - z^4 t_{1232})(1 - z^4 t_{1323})(1 - z^5 t_{12123}) \dots \\ &= 1 - z^2 t_{12} - z^2 t_{23} - z^2 t_{31} - z^3 t_{123} - z^3 t_{132} \\ &\quad - z^4 [(t_{1213} - t_{12} t_{13}) + (t_{1232} - t_{12} t_{23}) + (t_{1323} - t_{13} t_{23})] \\ &\quad - z^5 [(t_{12123} - t_{12} t_{123}) + \dots] - \dots \end{aligned} \quad (44)$$

Again the terms that stay isolated are exactly the ones indicated by the topological zeta function. If the disks are placed in a symmetric arrangement then there are relations between the orbits and the zeta functions factorize and simplify in a beautiful manner to be explained in the next section.

## 4 Symmetries

Many dynamical systems of interest come equipped with symmetries. Continuous symmetries usually give rise to conserved quantities by Noether's theorem. Discrete symmetries provide relations between trajectories and can be used to decompose phase space and dynamics into irreducible subspaces, just as in the familiar case of a quantum system with symmetry where eigenvalues and eigenvectors can be determined for the invariant subspaces separately [6, 69, 70, 18, 71].

Basic to this is the observation that a discrete symmetry can act on an orbit in two ways: it can map the set of points making up the orbit into itself or it can map it into

a different set which then again is an orbit. In the latter case, the properties (actions, periods, stabilities) of the orbit are unchanged, so that some factors in (44) coincide.

The symmetry group of three circular disks arranged on the vertices of an equilateral triangle is  $C_{3v}$ , consisting of the identity  $e$ , two rotations  $C_3$  and  $C_3^2$  by  $2\pi/3$  and  $4\pi/3$  around the center and three reflections  $c_{12}$ ,  $c_{13}$  and  $c_{23}$  on symmetry lines (see Fig. 4). For instance, the rotations map the orbit  $\overline{12}$  into  $\overline{13}$  and  $\overline{23}$ . Any one reflection maps  $\overline{123}$  into  $\overline{132}$  and so forth. Taking just one representative of every degenerate class of orbits, the zeta function (44) becomes

$$\begin{aligned}
1/\zeta &= (1 - z^2 t_{12})^3 (1 - z^3 t_{123})^2 (1 - z^4 t_{1213})^3 \\
&\quad (1 - z^5 t_{12123})^6 (1 - z^6 t_{121213})^6 (1 - z^6 t_{121323})^3 \dots \\
&= 1 - 3z^2 t_{12} - 2z^3 t_{123} - 3z^4 (t_{1213} - t_{12}^2) - 6z^5 (t_{12123} - t_{12} t_{123}) \\
&\quad - z^6 (6 t_{121213} + 3 t_{121323} + t_{12}^3 - 9 t_{12} t_{1213} - t_{123}^2) \\
&\quad - 6z^7 (t_{1212123} + t_{1212313} + t_{1213123} + t_{12}^2 t_{123} - 3 t_{12} t_{12123} - t_{123} t_{1213}) \\
&\quad - 3z^8 (2 t_{12121213} + t_{12121313} + 2 t_{12121323} + 2 t_{12123123} \\
&\quad + 2 t_{12123213} + t_{12132123} + 3 t_{12}^2 t_{1213} + t_{12} t_{123}^2 \\
&\quad - 6 t_{12} t_{121213} - 3 t_{12} t_{121323} - 4 t_{123} t_{12123} - t_{1213}^2) - \dots
\end{aligned} \tag{45}$$

A further reduction may be achieved by considering orbits whose trajectories are mapped into themselves under a symmetry operation. Then the orbit can actually be subdivided into irreducible segments, the full orbit being a combination of several segments. Similarly, the plane may be divided into a fundamental domain (Fig. 4) and its images under the symmetry operations. One can then define a new code based on the group elements needed to map a trajectory back onto the fundamental domain. The fundamental operation is a reflection every time the particle hits the boundary of the fundamental domain. If this is the only reflection between two collisions with the disk, a symbol 0 is assigned, but if two are needed (corresponding to a rotation), then the symbol is 1. This new code turns out to be binary without any restrictions. In Table 2 some orbits and their binary and ternary codes are listed.

For instance, the orbit  $\overline{123}$  is invariant under the rotations  $C_3$  and  $C_3^2$ . It can be pieced together from three identical segments 12, 23 and 31, mapped into each other by a rotation. Under a reflection, this orbit goes over into  $\overline{321}$ , which is just the time reversed orbit and therefore has the same symmetry. Its contribution to the zeta function can thus be written

$$(1 - t_{123})^2 = (1 - t_1^3)^2, \tag{46}$$

where the new label 1 comes from the fact that the orbit can be mapped back into the fundamental domain by a rotation. Similarly, the orbit  $\overline{12}$  is invariant under the reflection  $\sigma_{12}$ , so it can be pieced together from two segments 12 and 21. Application of the rotation produces two more orbits  $\overline{23}$  and  $\overline{31}$ . Its contribution to the zeta function can thus be written

$$(1 - t_{12})^2 = (1 - t_0^2)^3. \quad (47)$$

Then there are orbits without any symmetry relations, which have multiplicity 6. Finally, there are orbits related by time reversal symmetry but no other geometrical symmetry—only one member needs to be computed, which then enters with multiplicity 12.

The transfer operator is a linear operator and can therefore be decomposed into a direct sum of its irreducible representations, implying a factorization of zeta functions into products of zeta functions for the irreducible subspaces. An explicit construction of the transfer matrix based on the irreducible segments of an orbit is possible, but not necessary. Of interest are determinants, for which there is an expression involving traces only,

$$\begin{aligned} \det(1 + M) = & 1 + \operatorname{tr} M + \frac{1}{2} \left( (\operatorname{tr} M)^2 - \operatorname{tr} M^2 \right) \\ & + \frac{1}{6} \left( (\operatorname{tr} M)^3 - 3 (\operatorname{tr} M)(\operatorname{tr} M^2) + 2 \operatorname{tr} M^3 \right) \\ & + \cdots + \frac{1}{d!} \left( (\operatorname{tr} M)^d - \cdots \right). \end{aligned} \quad (48)$$

$d$  is the dimension of the representation. Since  $M$  is essentially a matrix representation of the group element under which the orbit is invariant, its traces are given by the characters  $\chi_\alpha(\mathbf{g}) = \operatorname{tr} D_\alpha(\mathbf{g})$ , listed in standard tables[72]. In terms of characters, we then have for the 1-dimensional representations

$$\det(1 - D_\alpha(\mathbf{g})t) = 1 - \chi_\alpha(\mathbf{g})t, \quad (49)$$

and for the 2-dimensional representations

$$\det(1 - D_\alpha(\mathbf{g})t) = 1 - \chi_\alpha(\mathbf{g})t + \frac{1}{2} \left( \chi_\alpha(\mathbf{g})^2 - \chi_\alpha(\mathbf{g}^2) \right) t^2. \quad (50)$$

Specifically, for the case of three symmetrically arranged disks and  $C_{3v}$  symmetry, one has two one-dimensional irreducible representations, symmetric and antisymmetric under reflections, denoted  $A_1$  and  $A_2$ , and two degenerate two-dimensional representations of

mixed symmetry, denoted  $E$ . The contribution of an orbit with symmetry  $g$  to the  $1/\zeta$  Euler product (48) factorizes according to

$$\det(1 - D(\mathbf{g})t) = (1 - \chi_{A_1}(\mathbf{g})t)(1 - \chi_{A_2}(\mathbf{g})t) \left(1 - \chi_E(\mathbf{g})t + \chi_{A_2}(\mathbf{g})t^2\right)^2. \quad (51)$$

Using the character table for the  $C_{3v}$  group,

$C_{3v}$	$A_1$	$A_2$	$E$
$e$	1	1	2
$C_3, C_3^2$	1	1	-1
$\sigma_v$	1	-1	0

one finds the following contributions from cycles:

$$\begin{array}{llll}
\mathbf{g}_{\tilde{p}} & A_1 & A_2 & E \\
e : & (1 - t_{\tilde{p}})^6 & = & (1 - t_{\tilde{p}})(1 - t_{\tilde{p}})(1 - 2t_{\tilde{p}} + t_{\tilde{p}}^2)^2 \\
C_3, C_3^2 : & (1 - t_{\tilde{p}}^3)^2 & = & (1 - t_{\tilde{p}})(1 - t_{\tilde{p}})(1 + t_{\tilde{p}} + t_{\tilde{p}}^2)^2 \\
\sigma_i : & (1 - t_{\tilde{p}}^2)^3 & = & (1 - t_{\tilde{p}})(1 + t_{\tilde{p}})(1 + 0t_{\tilde{p}} - t_{\tilde{p}}^2)^2,
\end{array} \quad (52)$$

where  $\tilde{p}$  denotes the symmetry reduced binary code for the segments of the orbit.

The outcome of this exercise is that the factorization within the  $A_1$  subspace is given by that of the binary zeta function (41), and that the one for the  $A_2$  case is similar, except that the contributions from orbits with an odd number of 0's change sign. More interesting is the zeta function for the  $E$  subspace, which contains a different pattern of terms,

$$\begin{aligned}
1/\zeta_E &= (1 + zt_1 + z^2t_1^2)(1 - z^2t_0^2)(1 + zt_{100} + z^2t_{100}^2)(1 - z^2t_{10}^2) \\
&\quad (1 + zt_{1001} + z^2t_{1001}^2)(1 + zt_{10000} + z^2t_{10000}^2) \\
&\quad (1 + zt_{10101} + z^2t_{10101}^2)(1 - z^2t_{10011})^2 \dots \\
&= 1 + zt_1 + z^2(t_1^2 - t_0^2) + z^3(t_{001} - t_1t_0^2) \\
&\quad + z^4 \left[ t_{0011} + (t_{001} - t_1t_0^2)t_1 - t_{01}^2 \right] \\
&\quad + z^5 \left[ t_{00001} + t_{01011} - 2t_{00111} + (t_{0011} - t_{01}^2)t_1 + (t_1^2 - t_0^2)t_{100} \right] + \dots \quad (53)
\end{aligned}$$

Similar decompositions hold for other symmetry groups[70, 71].

## 5 The three disk system

The formal developments of the previous sections will now be applied to the three disk billiard[59, 18, 61, 60, 73]. This system is ideally suited to test the methods since a good symbolic dynamics is known and tuning of a parameter allows one to study the transition from an open strongly chaotic system to a bounded one.

### 5.1 Periodic orbits

The example we will consider is motion of a point particle in the plane with three circles removed. The system is characterized by the ratio  $d/R$  of the distance  $d$  between the centers of the disks and their radius  $R$ . If the distance between the circles is larger than the radius,  $d/R > 2$ , then all of the plane is classically accessible and we have a scattering geometry. If on the other hand the three disks touch then they enclose a tipped region which we will refer to as the bounded billiard.

The classical dynamics of this system reduces to an exercise in geometry. Several coordinate systems are possible: either position along the circumference of the disks and parallel momentum or position and length of the segment between any two collisions[60, 74] or scattering coordinates, i.e. impact parameter and ingoing angle. More important is the choice of a numerically stable routine to find the orbit[74, 75]. Drawing on general experience in numerical mathematics a multipoint shooting method suggests itself. All intermediate point trajectory are allowed to vary, so that for an orbit of symbol length  $n$  one has  $2n$  variables. A Newton-Raphson iteration will typically converge very rapidly.

### 5.2 Convergence of the trace formula

The exponent in the semiclassical expression for the density of states (11) becomes for billiards  $S(E)/\hbar = Lk$  with  $k = \sqrt{2mE}/\hbar$  the wavenumber and  $L$  the geometrical length of the paths. All lengths can be taken relative to the radius of the disks. The semiclassical limit  $\hbar \rightarrow 0$  corresponds to  $k \rightarrow \infty$ .

In many systems, the number of periodic orbits in (11) increases and their weight decreases exponentially with period. The balance between these effects determines convergence[11, 12]. For billiards, the period of an orbit is proportional to its length, so that one has equivalent statements for the proliferation of orbits with increasing geometrical length. The absolute convergence of the series (11) is determined by the sum over absolute

values. Allowing for complex wavenumbers  $k = k_r + is$ , this becomes

$$\sum_p \sum_{r=1}^{\infty} \frac{L_p}{|\det(1 - M_p^r)|^{1/2}} e^{-rL_p s}. \quad (54)$$

This expression will converge for sufficiently large  $s$ , but will diverge for small  $s$ . As we are interested in the asymptotic behaviour for long orbits, we can replace  $\det(1 - M_p^r) \approx |\Lambda_p|^r$ , where  $|\Lambda_p|$  is the expanding eigenvalue of  $M_p$ . Then

$$\begin{aligned} \sum_p \sum_{r=1}^{\infty} L_p |\Lambda_p|^{-r/2} e^{-rsL_p} &= \sum_p L_p \frac{|\Lambda_p|^{-1/2} e^{-sL_p}}{1 - |\Lambda_p|^{-1/2} e^{-sL_p}} \\ &= \sum_p \frac{\partial}{\partial s} \log \left( 1 - |\Lambda_p|^{-1/2} e^{-sL_p} \right) \\ &= \frac{\partial}{\partial s} \log \zeta^{-1}(s) \end{aligned} \quad (55)$$

with the zeta function

$$1/\zeta = \prod_p \left( 1 - |\Lambda_p|^{-1/2} e^{-sL_p} \right). \quad (56)$$

This is yet another example of a dynamical zeta function, where the weights assigned to an orbit are  $t_p = |\Lambda_p|^{-1/2} e^{-sL_p}$ . The abscissa of convergence then emerges as a zero of this zeta function.

Fig. 5 shows  $-s_0$ , the negative of the abscissa of absolute convergence. This representation was chosen because of the similarity between  $-s_0$  and the classical escape rate  $\gamma$ , to be discussed in section 6.2. One curve was calculated using only the contributions from the fixed points in a cycle expanded form of (56), i.e. it shows the zero of

$$1 - |\Lambda_0|^{-1/2} e^{-sL_0} - |\Lambda_1|^{-1/2} e^{-sL_1}. \quad (57)$$

For the second curve the contributions

$$- |\Lambda_{01}|^{-1/2} e^{-sL_{01}} + |\Lambda_0 \Lambda_1|^{-1/2} e^{-s(L_0 + L_1)} \quad (58)$$

from the period two orbit have been included. Both curves agree well for  $d/R > 5$ . For sufficiently separated disks the abscissa of absolute convergence is negative, indicating convergence of the trace formula along the real axis. Near  $d/R \approx 2.8$  the curve crosses the real axis and approaches  $\approx 1.5$  for the closed billiard  $d/R \rightarrow 2$ .

The higher order zeta functions  $1/\zeta_j$  in the Selberg Zeta function contain more powers of  $\Lambda^j$ , so that their abscissa of convergence satisfy  $s_0^{(j)} < s_0^{(j-1)} < \dots < s_0$ . Since none of these functions can have zeros in the half plane  $\text{Im } k > s_0^{(j)}$ , the resonances closest to the real axis in the interval  $s_0^{(1)} < \text{Im } k < s_0^{(0)}$  come from  $1/\zeta_0$  alone. If  $s_0^{(0)} < 0$ , that is for  $d/R > 2.8$  then all resonances are semiclassically bounded away from the real axis. This gap has previously been identified by Gaspard[73].

### 5.3 Scattering resonances

Scattering processes can be described using the  $S$ -matrix. For the three disk system, the explicit expressions of the outgoing waves in terms of the ingoing waves using the scattering matrix have been given by Gaspard[73]. Resonances are related to complex zeros of  $\text{tr } S^\dagger \frac{dS}{dE}$ , which is the extension of the density of states to scattering systems[76]. It therefore is given by Gutzwiller's sum over classical periodic orbits, eq (11) with  $A = 1$ .

As discussed in section 4 on symmetries, the Selberg zeta function factorizes into three infinite products for the three subspaces of the symmetry group  $C_{3v}$  of the three disks. In the symmetry reduced symbolic code, the cycle expansion for the  $A_1$  subspace is given by the cycle expansion for a complete binary code, eq (41). Using all periodic orbits up to symbol length 5, in total 14 orbits, one finds the resonance spectrum (complex zeros) shown in Fig. 6. Evidently, the semiclassical calculations agree well with the quantum results. Also, almost all resonances are below the limit[73] predicted from the semiclassical calculations. That the two resonances with smallest real part are above the semiclassical limit is one of the deviations to be expected in the deep quantum regime.

### 5.4 Convergence of the cycle expansion

In recent years beautiful arguments for the convergence of the cycle expanded zeta function in the realm of semiclassics have been developed. Most important are attempts to obtain quantization conditions from a scattering matrix[24, 25, 26]. The basic observation is that for finite Planck's constant only a few scattering channels are open so that upon neglect of evanescent waves one deals with a finite scattering matrix. Therefore, the expansion of  $\det(1 - S)$  in a series in  $\text{tr } S^n$  as in eq (48) terminates. A different argument[27, 28] speculates about the existence of a Riemann Siegel relation and a bootstrapping of the contributions from longer orbits. A Riemann Siegel relation also holds within the scattering matrix formulation.

However, from a general point of view, the cycle expanded product should converge because of the compensations induced by approximations of long orbits from short ones[14, 15, 16]. In its most primitive form, the compensation argument applies to terms in eq (41) of the form  $t_{a^k b} - t_a t_{a^{k-1} b}$ , involving a long orbit  $a^k b$  and two approximands  $a$  and  $a^{k-1} b$ . This orbit is a periodic approximation to an orbit homoclinic to  $a$ . Substituting

the form of  $t_{a^k b}$  from eq (20) for  $j = 0$ , one finds

$$t_{a^k b} - t_a t_{a^{k-1} b} = t_{a^k b} \left( 1 - e^{i(S_a + S_{a^{k-1} b} - S_{a^k b})/\hbar} e^{-i\pi(\mu_a + \mu_{a^{k-1} b} - \mu_{a^k b})/2} \left| \frac{\Lambda_a \Lambda_{a^{k-1} b}}{\Lambda_{a^k b}} \right|^{-1/2} \right). \quad (59)$$

Because of our definition of the code in terms of selfconjugate points (section 3.2) the Maslov indices cancel,  $\mu_a + \mu_{a^{k-1} b} - \mu_{a^k b} = 0$ . Furthermore, since with increasing  $k$ , segments of  $a^k b$  become closer to  $a$ , the differences in action and the ratio of the eigenvalues converge exponentially with the eigenvalue of the orbit  $a$ ,

$$S_a + S_{a^{k-1} b} - S_{a^k b} \approx \text{const} \Lambda_a^{-k} \quad (60)$$

$$|\Lambda_a \Lambda_{a^{k-1} b} / \Lambda_{a^k b}| \approx \exp(-\text{const} \Lambda_a^{-k}) \quad (61)$$

Expanding the exponentials one thus finds that this term in the cycle expansion is of the order of

$$t_{a^k b} - t_a t_{a^{k-1} b} \approx \text{const} \Lambda_a^{-k}. \quad (62)$$

The number of terms in every order of the cycle expansion is even larger than the number of periodic orbits[71]. However, the compensations reduce the size of the contributions from the periodic orbits, inducing convergence. In the case of the three disks, compensations should be best for  $k = 0$  since one then does not have to worry about phases. As Fig. 7 shows, compensation is very good for  $d/R = 6$  and  $d/R = 3$ . What changes as one approaches the closed billiard  $d/R = 2$  is that the convergence is no longer as rapid and that pruning and missing orbits cause non monotonic variations (see below).

The above discussion also shows that with increasing energy more orbits are needed to obtain convergence: since the actions increase with energy, so do their differences. But if the differences become larger than  $O(\hbar)$ , it is no longer permitted to expand the exponentials and these terms have to be kept. However, for sufficiently long orbits, the compensations will again take place.

## 5.5 Eigenvalues for the bounded three disk billiard

Turning to the bounded billiard, one has to worry about additional problems associated with pruning of orbits. As the disks are moved closer, some orbits annihilate and disappear[61]. For instance the orbits  $\overline{000001}$  and  $\overline{0000011}$  exist for  $d/R > 2.016\dots$  only. Other orbits in the family  $\overline{0^n 1}$  and  $\overline{0^n 11}$  with  $n > 5$  vanish earlier. In addition to these,

the orbit  $\bar{0} = \bar{12}$  vanishes when the disks touch. These are the only pruning rules for orbits of period  $< 10$ .

As the disks move closer together, one would expect the resonances to move up towards the real axis, lining up on it for the closed system. The numerical calculations show this behaviour only approximately. Including all orbits up to length 10 one finds that the resonances lie near the real axis, but not exactly on it[61]. To remedy this, one can speculate about the existence of a functional relation for the Selberg zeta function which would put it on the real axis[24, 28].

The existence of a functional equation is suggested by the behaviour of the quantum mechanical integrated density of states  $N(E)$ : it is a piecewise constant function that jumps by 1 at every eigenvalue. To derive a semiclassical expression for this note that the smooth density of states in eq (11) can be written as the logarithmic derivative,

$$\rho_0(E) = -\frac{1}{\pi} \frac{\partial}{\partial E} \log \left( e^{-i\pi N_0} \right), \quad (63)$$

with

$$N_0(E) = \int dE \rho_0(E) \quad (64)$$

the integrated smooth density of states. Together with the Selberg Zeta function (18), (19) one finds

$$\rho(E) = -\frac{1}{\pi} \frac{\partial}{\partial E} \log \left( e^{-i\pi N_0} Z(E) \right) \quad (65)$$

or for the integrated density of states

$$N(E) = -\frac{1}{\pi} \log \left( e^{-i\pi N_0} Z(E) \right) \quad (66)$$

A piecewise constant function can be obtained if the argument of the logarithm is real. Then  $N(E)$  is constant inbetween zeros and jumps by one, if the argument has a simple zero, for then the phase jumps by  $\pi$ . Therefore, semiclassical approximations to eigenvalues can be obtained as the zeros of

$$D(E) = e^{-i\pi N_0} Z(E). \quad (67)$$

This expression is very close to the functional determinant  $\det(E - E_i)$ , (see, e.g., Ref. [77]).

For the billiard, the mean integrated density of states is given by the Weyl expansion[42], containing the area, circumference and curvature of the billiard plus a term from the singular tip at the touching point of the disks. The contributions from the periodic orbits to

the density of states in the  $A_1$  symmetry can be expanded as in eq (41). Fig. 8 shows two approximations to  $D(k)$  vs.  $k$  for the three disk billiard, one involving all orbits up to length 2 and length 3, respectively. The overall agreement is good and most eigenvalues are resolved. Again there are (quantum) deviations for small  $k$ .

## 6 Classical periodic orbit theory

When transferred to classical mechanics, the manipulations that lead from the quantum propagator to the response function yield an expression for the classical spectrum in terms of periodic orbits[78]. This is useful in interpreting resonances in classical correlation functions. In addition, these classical expressions contain information on classical escape rates in open systems[81] and the Ozorio de Almeida-Hannay sum rule in bounded systems[82].

### 6.1 The classical trace formula and associated zeta function

Without much difficulty one can carry over Gutzwiller's arguments[6, 7] from quantum mechanics to classical mechanics and derive a periodic orbit representation for the classical propagator. Starting point is Liouville's equation for phase space densities  $f$ ,

$$\dot{f} = -i\mathcal{L}f, \quad (68)$$

with the formal solution

$$f_t = e^{-i\mathcal{L}t} f_0. \quad (69)$$

The equivalent of a Green's function may be defined by Fourier transform in time,

$$G_{cl} = \int dt e^{i\omega t} e^{-i\mathcal{L}t}, \quad (70)$$

and the trace of Green's function then gives the density of states,

$$\rho_{cl} = \text{tr } G_{cl} = \sum_i \frac{1}{\omega - \omega_i}. \quad (71)$$

The spectrum of an ergodic system[83, 84] has one eigenvalue at  $\omega = 0$ , connected with the invariant measure, superimposed on a continuum. This continuum will show resonances which can be thought of as complex poles  $\omega_i$ .

The calculation proceeds from an expression of the classical propagator as an integral operator,

$$f_t(\mathbf{x}) = \int d\mathbf{q} \delta(\mathbf{x} - \mathbf{q}_t) f_0(\mathbf{q}), \quad (72)$$

where  $\mathbf{q}_t$  denotes the point  $\mathbf{q}$  propagated forward in time. Upon taking the trace, the delta function singles out orbits that return to their starting point: periodic orbits. Thus the delta function only gives a contribution whenever  $t$  equals a period  $T_p$ . Changing to a coordinate system along the orbit and perpendicular to it one can do the perpendicular integration, resulting in a factor  $1/\det(1 - M_p)$ , and the integration along the orbit, resulting in the period. In view of the delta function the Fourier transform in time is easily done, leading to an expression

$$\rho_{cl} = \sum_p \sum_{r=1}^{\infty} \frac{T_p}{\det(1 - M_p^r)} e^{ir\omega T_p}, \quad (73)$$

which by manipulations similar to the ones in section 2.2 can be expressed as the logarithmic derivative of the zeta function

$$Z_{cl}(\omega) = \prod_{k=0}^{\infty} \prod_p (1 - |\Lambda_p|^{-1} \Lambda_p^{-k} e^{i\omega T_p})^{k+1}, \quad (74)$$

where the origin of the power  $k + 1$  may be traced to the fact that in contrast to the quantum case one has a full determinant rather than a square root in the denominator.

## 6.2 Escape rates and sum rules

I shall not give a complete discussion of the classical periodic orbit expression and its use in determining resonances[79, 80], except for a discussion of the significance of a zero at real  $s$ .

Consider first a scattering system such as the arrangement of three non-touching disks. One can then ask for the time a particle will spend in the central region[81]. For this hyperbolic system the distribution of these trapping times is exponential, and can be characterized by a mean trapping time  $\gamma^{-1}$  or its inverse, the escape rate  $\gamma$ . One method to calculate  $\gamma$  makes use of trapped periodic orbits. Roughly speaking, if a trajectory makes  $n$  bounces, then it will be close to some periodic orbit of that period. The orbit is exponentially unstable and the probability of staying near it is given by the inverse of the expanding eigenvalue. The average over all periodic points, including multiple traversals, then is

$$\sum_p \sum_{r=1}^{\infty} T_p |\Lambda_p|^{-r} e^{-T_p s r}, \quad (75)$$

which is exactly of the form of the semiclassical expression above, with the exception that now a full eigenvalue appears rather than its square root. Therefore, by manipulations similar to the ones in eq (55), one can write this as the logarithmic derivative of the zeta function

$$1/\zeta = \prod_p \left(1 - |\Lambda_p|^{-1} e^{-T_p s}\right). \quad (76)$$

Using cycle expansions up to  $n = 1$  and  $n = 2$ , respectively, one finds the curves shown in Fig. 9. The agreement between the two curves is an indication of the rapid convergence of the cycle expansion. Also shown are the results of a classical Monte Carlo simulation of Gaspard[60].

There is a direct connection between the escape rate[81] and the classical sum rule proposed by Hannay and Ozorio de Almeida[82]. According to one formulation (see in particular section 17.7 of Gutzwiller's book[6]), the sum

$$\sum_{T_p < T} \frac{T_p}{\det(1 - M_p)} \approx 1, \quad (77)$$

so that the set of periodic orbits approximates the phase space measure in the sense that every average over phase space can be expressed as an average over periodic orbits. Rather than defining a set of orbits by their periods, one can also take all periodic orbits of a fixed symbol length. Then the equivalent statement is that

$$\sum_{(n)} \frac{T_p}{\det(1 - M_p)} \approx 1. \quad (78)$$

This may be expressed as a logarithmic derivative of a zeta function by multiplication with  $z^n$  and summation over  $n$ . That the sum approaches a constant then means that the zeta function

$$1/\zeta = \prod_p (1 - |\Lambda_p|^{-1} z^{n_p}) \quad (79)$$

has a zero for  $z = 1$ . But this is just the escape rate zeta function eq (76) for  $s = 0$ , so that a vanishing escape rate indicates that the periodic orbits represent the invariant phase space density (in hyperbolic systems).

## 7 Matrix elements

In this final section, I will discuss the derivation of a zeta function for the diagonal matrix elements and indicate the extension to off-diagonal matrix elements[36].

## 7.1 Diagonal matrix elements

As discussed in section 2.1, the final expression for  $\text{tr} GA$  with some sufficiently smooth observable  $A$  becomes:

$$\begin{aligned} \rho_A(E) &= \int \frac{d\mathbf{q}d\mathbf{p}}{h^N} A(\mathbf{q}, \mathbf{p}) \delta(E - H(\mathbf{q}, \mathbf{p})) \\ &+ \text{Im} \frac{i}{\pi\hbar} \sum_p \sum_{r=1}^{\infty} \frac{A_p}{|\det(M_p^r - 1)|^{1/2}} e^{(iS_p(E)/\hbar - i\pi\mu/2)r}, \end{aligned} \quad (80)$$

where

$$A_p = \int_0^{T_p} dt A(\mathbf{q}_p(t), \mathbf{p}_p(t)). \quad (81)$$

The derivation of a zeta function for matrix elements is similar to the calculation in section 2.2, except for one step. One first arrives at

$$R_{A,osc} = \frac{1}{\pi\hbar} \sum_p \sum_{j=0}^{\infty} \frac{A_p \tilde{t}_p^{(j)}}{1 - \tilde{t}_p^{(j)}}, \quad (82)$$

where  $\tilde{t}_p^{(j)} = e^{iS_p/\hbar - i\mu_p\pi/2} |\Lambda_p|^{-1/2} \Lambda_p^{-j}$ . In the case of the density of states, the observable is  $A = 1$  and the prefactor  $A_p = T_p = \partial S/\partial E$  so that one can immediately write the quotient in (16) as a logarithmic derivative and thus arrive at the zeta functions. Here, one may proceed similarly after introducing an auxiliary variable  $\gamma$  and an extended  $t_p^{(j)} = e^{-\gamma A_p} \tilde{t}_p^{(j)}$ . Since  $\tilde{t}_p^{(j)} = t_p^{(j)}(\gamma = 0)$  and  $A_p \tilde{t}_p^{(j)} = \partial t_p^{(j)} / \partial \gamma|_{\gamma=0}$ , one can write

$$R_{A,osc} = \frac{i}{\pi\hbar} \sum_p \sum_{j=0}^{\infty} \frac{\partial}{\partial \gamma} \log(1 - t_p^{(j)}) \Big|_{\gamma=0} \quad (83)$$

and thus finally

$$R_{A,osc} = \frac{i}{\pi\hbar} \frac{\partial}{\partial \gamma} \ln Z(\gamma, E) \Big|_{\gamma=0} \quad (84)$$

with the extended Selberg type product

$$Z(\gamma, E) = \prod_p \prod_{j=0}^{\infty} (1 - e^{-\gamma A_p} e^{iS_p/\hbar - i\mu_p\pi/2} |\Lambda_p|^{-1/2} \Lambda_p^{-j}). \quad (85)$$

For  $\gamma = 0$  this dynamical zeta function coincides with the Selberg Zeta function  $Z_s(E)$  for the spectral density  $\rho(E)$ ,

$$Z_s(E) = Z(\gamma = 0, E). \quad (86)$$

Eq (85) may again be evaluated using the cycle expansion. Consider the case of a hyperbolic system with complete binary symbolic dynamics. Labelling the contributions from the periodic orbits by their symbolic code, one has to consider products of the form

$$Z(\gamma, E) = (1 - t_0)(1 - t_1)(1 - t_{01})(1 - t_{001})(1 - t_{011}) \cdots, \quad (87)$$

which expand into

$$Z(\gamma, E) = 1 - t_0 - t_1 - (t_{01} - t_0 t_1) - (t_{001} - t_0 t_{01}) - (t_{011} - t_1 t_{01}) \cdots \quad (88)$$

Upon taking the derivative, one has

$$\begin{aligned} \frac{\partial Z(\gamma, E)}{\partial \gamma} &= A_0 t_0 + A_1 t_1 + [A_{01} t_{01} - (A_0 + A_1) t_0 t_1] \\ &\quad + [A_{001} t_{001} - (A_0 + A_{01}) t_0 t_{01}] \\ &\quad + [A_{011} t_{011} - (A_1 + A_{01}) t_1 t_{01}] \cdots \end{aligned} \quad (89)$$

The suggestive argument for convergence (section 5.4) is that a long orbit  $t_{ab}$  can be decomposed into shorter ones (labelled  $a$  and  $b$ ), which shadow it; therefore, the term  $t_{ab} - t_a t_b$  is small. However, the same can be expected of the observable: if the short orbits  $a$  and  $b$  are close to  $ab$ , then  $A_{ab}$  should also be close to  $A_a + A_b$  and the convergence properties of the above cycle expansion can be expected to be the same as the ones for the density of states.

## 7.2 Correlation functions

A similar result may be obtained for correlation functions. All one has to note is that in the semiclassical limit the time evolution of the operator  $B$  is given by the classical observable  $B$  at the time evolved positions. Therefore, one obtains correlation functions if the observable  $A(\mathbf{p}, \mathbf{q})$  is replaced by  $B(\mathbf{p}(t), \mathbf{q}(t))C(\mathbf{p}, \mathbf{q})$ , where  $(\mathbf{p}(t), \mathbf{q}(t))$  denotes the point reached by a trajectory starting at time  $t = 0$  from  $(\mathbf{p}, \mathbf{q})$ . The final result is exactly as above, except that  $A_p$  is replaced by

$$A'_p = \int_0^{T_p} dt' B(\mathbf{q}(t' + t), \mathbf{p}(t' + t)) C(\mathbf{q}(t'), \mathbf{p}(t')), \quad (90)$$

the correlation function of  $B$  and  $C$  along the periodic orbit. The first term, the contribution of paths of zero length, becomes the classical correlation function.

Quantum mechanically,  $\text{tr } G B_t C$  evaluates to

$$\text{tr } G B_t C = \sum_n \frac{\langle n | B_t C | n \rangle}{E - E_n}, \quad (91)$$

where

$$\langle n|B_t C|n\rangle = \sum_m \langle n|B|m\rangle \langle m|C|n\rangle e^{i(E_n - E_m)t/\hbar}; \quad (92)$$

one therefore expects the semiclassical expression to have poles at the eigenenergies, with residues the matrix elements  $\langle n|B_t C|n\rangle$ .

### 7.3 Periodic orbit spectroscopy

The developments in the previous section pave the way for what one may call ‘periodic orbit spectroscopy’[85]. A Fourier transform of spectra in terms of a suitable scaling variable very often reveals sharply defined peaks, which according to semiclassics can be assigned to periodic orbits. The most prominent example of this is hydrogen in a magnetic field, where the comparison between classical and quantum mechanics has been pushed very far[8, 9, 86].

The formula for autocorrelation functions should be useful in describing Rydberg-Rydberg transitions. Calculations by Zeller[87] for hydrogen in a magnetic field have in fact revealed periodic orbit structures for transitions between highly excited states. A quantitative comparison would be highly desirable.

As an application outside atomic physics, Wilkinson[34] has suggested to apply the above formula to conductance problems, since the conductance is related to the Fourier transform of a correlation function by the Kubo Greenwood formula[88, 89]. This relation may be useful for the AC behaviour, but must be expected to fail in the DC limit since it does not describe correctly the infinite time limit of the correlation functions[36].

Periodic orbits also figure prominently in recent interpretations of the spectra of small molecules[90]. Their presence becomes plausible via the classical periodic orbit formula. It would be interesting to identify semiclassical corrections to this.

## 8 Final remarks

Evidently, periodic orbit expansions provide a powerful tool for all kinds of calculations in classical and semiclassical mechanics. Almost all quantities of interest can be expressed in terms of periodic orbits or, more precisely, traces of transfer matrices. The cycle expansion with its arrangement of periodic orbits into compensating groups provides a numerically efficient and convergent method to evaluate periodic orbit expressions.

The tests presented here and others have aimed at verifying the semiclassical approximation level by level. This is mainly of theoretical interest, to strengthen confidence and explore the range of validity and reliability of the Gutzwiller trace formula, which after all is derived using many approximations. The indications are that it is a bona fide semiclassical theory, which shows large deviations from exact quantum calculation in the quantum domain of small wavenumbers, but better agreement at higher energies in the truly semiclassical regime. There still is the question of whether the present form of semiclassics can actually give the positions of resonances accurately to better than a mean spacing, considering that the propagator includes terms of order  $\hbar$  only, whereas the mean density of states is  $O(\hbar^2)$ . Indications are that the error will not be noticable until one gets to very high energies. However, it should be more important as the number of degrees of freedom increases.

On the practical side, this appears to be just a minor limitation. The strength of the semiclassical expressions is that they can explain long range correlations in the spectra, somewhat independent of the fine structure of the spectrum. The aim will be to calculate semiclassically from just a few periodic orbits the spectra of small molecules and to use this as a tool in analyzing spectra. The most prominent example of this class is hydrogen in a magnetic field, but currently some molecules are under investigation where such quantitative predictions may be possible as well.

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n	$M_n(N)$	$M_n(2)$	$M_n(3)$	$M_n(4)$
1	$N$	2	3	4
2	$N(N-1)/2$	1	3	6
3	$N(N^2-1)/3$	2	8	20
4	$N^2(N^2-1)/4$	3	18	60
5	$(N^5-N)/5$	6	48	204
6	$(N^6-N^3-N^2+N)/6$	9	116	670
7	$(N^7-N)/7$	18	312	2340
8	$N^4(N^4-1)/8$	30	810	8160
9	$N^3(N^6-1)/9$	56	2184	29120
10	$(N^{10}-N^5-N^2+N)/10$	99	5880	104754

Table 1. Number of prime cycles for various alphabets and grammars up to length 10. The first column gives the cycle length, the second the formula (28) for the number of prime cycles for complete  $N$ -symbol dynamics, columns three through five give the numbers for  $N = 2, 3$  and 4.

$\tilde{p}$	$p$	$\mathbf{g}_{\tilde{p}}$
0	1 2	$\sigma_{12}$
1	1 2 3	$C_3$
01	12 13	$\sigma_{23}$
001	121 232 313	$C_3$
011	121 323	$\sigma_{13}$
0001	1212 1313	$\sigma_{23}$
0011	1212 3131 2323	$C_3^2$
0111	1213 2123	$\sigma_{12}$
00001	12121 23232 31313	$C_3$
00011	12121 32323	$\sigma_{13}$
00101	12123 21213	$\sigma_{12}$
00111	12123	$e$
01011	12131 23212 31323	$C_3$
01111	12132 13123	$\sigma_{23}$
000001	121212 131313	$\sigma_{23}$
000011	121212 313131 232323	$C_3^2$
000101	121213	$e$
000111	121213 212123	$\sigma_{12}$
001011	121232 131323	$\sigma_{23}$
001101	121231 323213	$\sigma_{13}$
001111	121231 232312 313123	$C_3$
010111	121312 313231 232123	$C_3^2$
011111	121321 323123	$\sigma_{13}$

Table 2.  $C_{3v}$  correspondence between the binary labelled fundamental domain prime cycles  $\tilde{p}$  and the full 3-disk ternary  $\{1,2,3\}$  cycles  $p$ , together with the  $C_{3v}$  transformation that maps the end point of the  $\tilde{p}$  cycle into the irreducible segment of the  $p$  cycle. The degeneracy of  $p$  cycle is  $m_p = 6n_{\tilde{p}}/n_p$ . The shortest pair of the fundamental domain prime cycles related by time symmetry are the 6-cycles  $\overline{001011}$  and  $\overline{001101}$ .

## Figure captions

1. The three disk billiard. The trajectory can be labelled by its disk visitation sequence, viz. 1231312.
2. Construction of impact parameters for long collision sequences. The dashed lines indicate the interval in impact parameter leading to collisions with disk 1. Initial conditions in the two shaded intervals lead to collisions with 1 and 2 or 1 and 3, respectively.
3. Two orbits for hydrogen in a magnetic field in semiparabolic coordinates. The energy is  $+0.2 Ry$ . The self conjugate points are indicated. The four disk code of the two trajectories is 142124 and **14121214**, respectively. The collisions indicated in bold face are not immediately obvious in configuration space but clearly identified by the presence of two additional self conjugate points.
4. Symmetries of the three disk scattering system. Indicated are the three reflections  $\sigma_i$  across symmetry lines, the two rotations  $C_3$  and  $C_3^2$  around the center by  $\pm 2\pi/3$  and the fundamental domain (shaded).
5. The abscissa of absolute convergence for the system of three disks as a function of the distance/radius ratio  $d/R$ .
6. Some resonances of the  $S$ -matrix in the  $A_1$  subspace for  $d/R = 6$ . The crosses are the exact quantum results, the open circles the result from a semiclassical calculation involving all periodic orbits up to symbol length 5. Notice that all semiclassical resonances lie below the abscissa of absolute convergence,  $\text{Im } k_c = -0.123\dots$ , but that the first two quantum resonances lie above.
7. Convergence of the cycle expanded zeta function for the three disk system. The terms  $c_n$  contain all contributions from orbits and pseudo-orbits of length  $n$  (see eq (41)) at  $k = 0$ .
8. The functional determinant (67) for the closed three disk system including orbits of symbol length  $n = 2$  and  $n = 3$ . The dotted vertical lines indicate the positions of the exact quantum eigenvalues.
9. Classical escape rate  $\gamma$  as a function of the distance between the disks. The crosses are the results of a Monte Carlo simulation by Gaspard[60].